

Computers in Chemistry – Lecture IV

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1

Get this lecture online

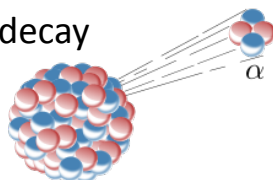
- Please go to: <http://qc.chem.nagoya-u.ac.jp>
- Click on “Teaching” (English website only, sorry!)
- Click on “PPT” link of “4.1 Lecture IV – Programming and problem solving”
userid: **qcguest**, password: **qcigf!**

3.1 Lecture III - Introduction to computer programming (PDF)
3.2 Assignment 3 (PDF)
3.3 Example programs: `hello.c` `hello.f`
4.1 Lecture IV - Programming and problem solving (PDF)
4.2 Assignment 4 (PDF)
4.3 Part of Chapter 1 by NL (English) (Japanese)
4.4 Example program: `fig1-8.f90` (Radioactive Decay)

2

Today's Lecture

- The “art” of programming and problem solving
- Five steps of program development
- A specific example: radioactive decay
- Flow charts
- Key concepts in FORTRAN 90

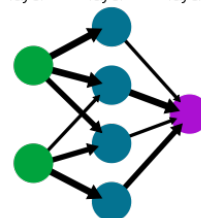


3

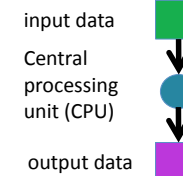
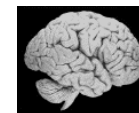
The “art” of programming

- Human brain and computer is **radically** different!

A simple neural network
input layer hidden layer output layer



Not digital: fuzzy logic (continuous spectrum within [0,1])



Digital: binary logic (only “off”=0 and “on”=1 state)

4

Five Steps of Program Development I

- Step 1: Problem Analysis and Specification
- Step 2: Data Organization and Algorithm Design
- Step 3: Program Coding (the act of writing a program)
- Step 4: Compilation, execution and testing
- Step 5: Program maintenance

5

Five Steps of Program Development II

- **Step 1: Problem Analysis and Specification**

Example Problem (from NL page 6, check English or Japanese PDF files):

How much Polonium 210 (most widely available isotope) remains after 180 days if 10 milligrams were available initially? Note that the half-life of Polonium 210 is ~140 days.

6

Five Steps of Program Development III

Step 1 (continued): Analyze the problem and formulate a specification of it.

Input: what information is given

Output: what information must be produced to solve the problem

Input: initial amount of ^{210}Po , half-life, time-period

Output: Amount remaining

7

Five Steps of Program Development IV

Step 2: Data Organization and Algorithm Design

Determine how to organize and store the data in the problem

Develop procedures to process the data and produce the required output. These **procedures are called algorithms**

Example for Data Organization:

Input variables: 1) InitialAmount, 2) HalfLife, 3) Time

Output variable: AmountRemaining

8

Five Steps of Program Development V

Step 2 (continued): Data Organization and Algorithm Design

Algorithm Design: What needs to be done?

1. Get values for InitialAmount, HalfLife, and Time
2. Compute the value of AmountRemaining using a mathematical formula
3. Display AmountRemaining

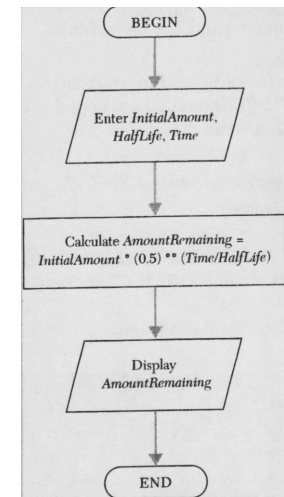
9

Five Steps of Program Development VI

Step 2 (continued): Data Organization and Algorithm Design

Express this by a **flow chart**:

1. Get values for InitialAmount, HalfLife, and Time
2. Compute the value of AmountRemaining using a mathematical formula
3. Display AmountRemaining



10

Five Steps of Program Development VII

Step 3: Program Coding (writing)

Usually, we use an editor to write a file that contains the program, such as “pico” (see lecture III)

In this case, **get the program from QC website** (Ctrl-Click and save):

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- 3.2 Assignment 3 (PDF)
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- 4.4 Example program: [fig1-8.f90](#) (Radioactive Decay)

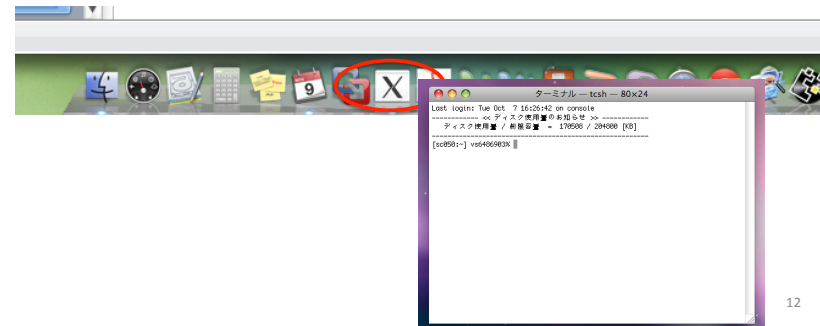
11

Five Steps of Program Development VIII

Step 3 (continued): Program Coding (writing)

Check that the program exists on your home directory (\$HOME):

Login to X-windows, which opens a terminal



12

Five Steps of Program Development IX

Step 3 (continued): Program Coding (writing)

Type “ls”: check that the program fig1-8.f90 exists in your directory.

Type “pico fig1-8.f90” which opens the pico editor with your file. If you are happy with this file, exit pico by <Ctrl-X>

13

Five Steps of Program Development IX

Step 4: Compilation, execution, and testing

Compile: Type “gfortran -o fig1-8.x fig1-8.f90” – this should produce no output if everything was successful.

Execute: Type “./fig1-8.x”

You will see:

Enter initial amount (mg) of substance, its half-life (days) and time (days) at which to find amount remaining:

14

Five Steps of Program Development X

Step 4 (continued): Compilation, execution, and testing

Enter answers and you will see:

10, 140, 180

Amount remaining = 4.101677 mg

Play with the input and output. For instance, the half-time of Cs 137 is ~30.2 years = 11023 days

This concludes today’s lecture.

15